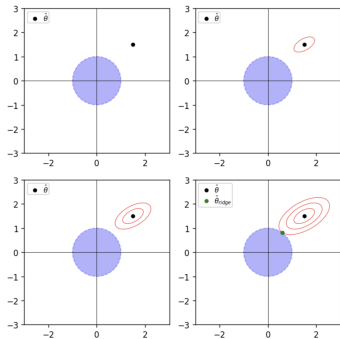


# Introduction to Machine Learning

## Regularization

## Ridge Regression



### Learning goals

- Regularized linear model
- Ridge regression /  $L_2$  penalty
- Understand parameter shrinkage
- Understand correspondence to constrained optimization

# REGULARIZATION IN LM

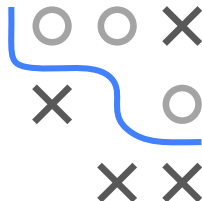
- Can also overfit if  $p$  large and  $n$  small(er)
- OLS estimator requires full-rank design matrix
- For highly correlated features, OLS becomes sensitive to random errors in response, results in large variance in fit
- We now add a complexity penalty to the loss:

$$\mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \sum_{i=1}^n \left( y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)} \right)^2 + \lambda \cdot J(\boldsymbol{\theta}).$$



# RIDGE REGRESSION / L2 PENALTY

Intuitive measure of model complexity is deviation from 0-origin; coeffs then have no or a weak effect. So we measure  $J(\theta)$  through a vector norm, shrinking coeffs closer to 0.



$$\begin{aligned}\hat{\theta}_{\text{ridge}} &= \arg \min_{\theta} \sum_{i=1}^n \left( y^{(i)} - \theta^T \mathbf{x}^{(i)} \right)^2 + \lambda \sum_{j=1}^p \theta_j^2 \\ &= \arg \min_{\theta} \|\mathbf{y} - \mathbf{X}\theta\|_2^2 + \lambda \|\theta\|_2^2\end{aligned}$$

Can still analytically solve this:

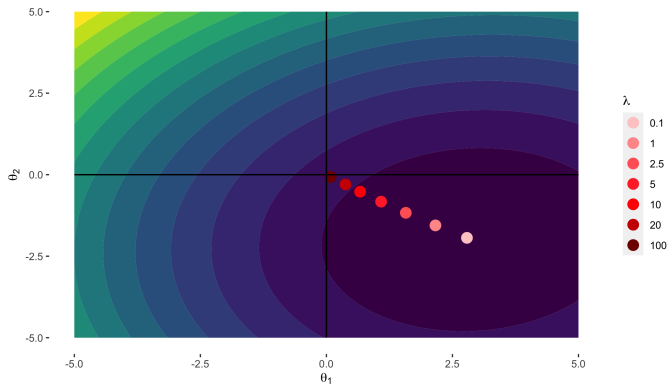
$$\hat{\theta}_{\text{ridge}} = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^T \mathbf{y}$$

Name: We add pos. entries along the diagonal "ridge" of  $\mathbf{X}^T \mathbf{X}$

# RIDGE REGRESSION / L2 PENALTY / 2

Let  $y = 3x_1 - 2x_2 + \epsilon$ ,  $\epsilon \sim N(0, 1)$ . The true minimizer is  $\theta^* = (3, -2)^T$ , with  $\hat{\theta}_{\text{ridge}} = \arg \min_{\theta} \|\mathbf{y} - \mathbf{X}\theta\|^2 + \lambda \|\theta\|^2$ .

Effect of L2 Regularization on Linear Model Solutions

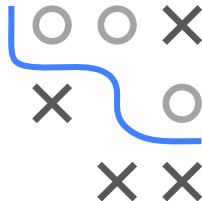
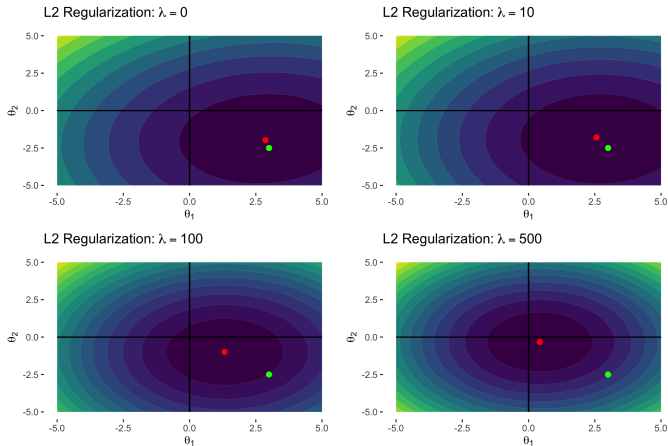


With increasing regularization,  $\hat{\theta}_{\text{ridge}}$  is pulled back to the origin (contour lines show unregularized objective).

# RIDGE REGRESSION / L2 PENALTY / 3

Contours of regularized objective for different  $\lambda$  values.

$$\hat{\theta}_{\text{ridge}} = \arg \min_{\theta} \|\mathbf{y} - \mathbf{X}\theta\|^2 + \lambda \|\theta\|^2.$$

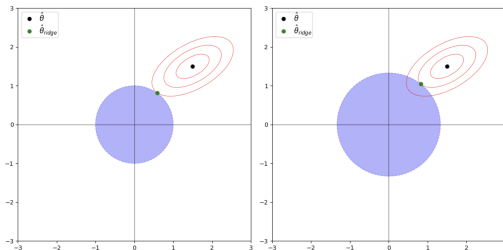


Green = true minimizer of the unreg.objective and red = ridge solution.

# RIDGE REGRESSION / L2 PENALTY / 4

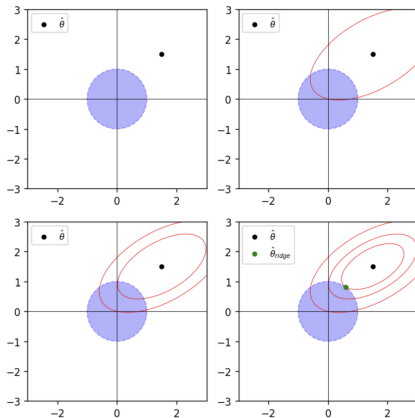
We understand the geometry of these 2 mixed components in our regularized risk objective much better, if we formulate the optimization as a constrained problem (see this as Lagrange multipliers in reverse).

$$\begin{aligned} \min_{\theta} \quad & \sum_{i=1}^n \left( y^{(i)} - f(\mathbf{x}^{(i)} | \theta) \right)^2 \\ \text{s.t.} \quad & \|\theta\|_2^2 \leq t \end{aligned}$$

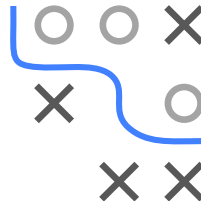


NB: There is a bijective relationship between  $\lambda$  and  $t$ :  $\lambda \uparrow \Rightarrow t \downarrow$  and vice versa.

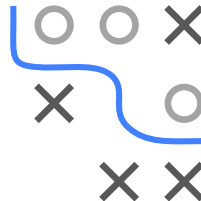
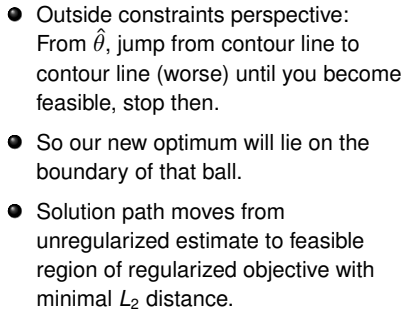
# RIDGE REGRESSION / L2 PENALTY / 5



- Inside constraints perspective: From origin, jump from contour line to contour line (better) until you become infeasible, stop before.
- We still optimize the  $\mathcal{R}_{\text{emp}}(\theta)$ , but cannot leave a ball around the origin.
- $\mathcal{R}_{\text{emp}}(\theta)$  grows monotonically if we move away from  $\hat{\theta}$  (elliptic contours).
- Solution path moves from origin to border of feasible region with minimal  $L_2$  distance.



## ©





## ©



- Here we can see entire solution path for ridge regression
- Cyan contours indicate feasible regions induced by different  $\lambda$ s
- Red contour lines indicate different levels of the unreg. objective
- Ridge solution (red points) gets pulled toward origin for increasing  $\lambda$



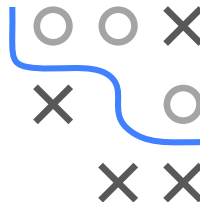
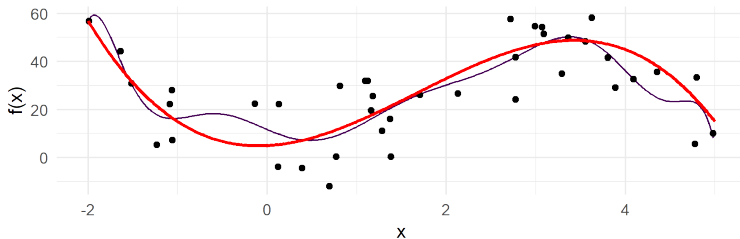
# EXAMPLE: POLYNOMIAL RIDGE REGRESSION

Consider  $y = f(x) + \epsilon$  where the true (unknown) function is  $f(x) = 5 + 2x + 10x^2 - 2x^3$  (in red).

Let's use a  $d$ th-order polynomial

$$f(x) = \theta_0 + \theta_1 x + \dots + \theta_d x^d = \sum_{j=0}^d \theta_j x^j.$$

Using model complexity  $d = 10$  overfits:



$\lambda$	$\theta_0$	$\theta_1$	$\theta_2$	$\theta_3$	$\theta_4$	$\theta_5$	$\theta_6$	$\theta_7$	$\theta_8$	$\theta_9$	$\theta_{10}$
0.00	12.00	-16.00	4.80	23.00	-5.40	-9.30	4.20	0.53	-0.63	0.13	-0.01
10.00	5.20	1.30	3.70	0.69	1.90	-2.00	0.47	0.20	-0.14	0.03	-0.00
100.00	1.70	0.46	1.80	0.25	1.80	-0.94	0.34	-0.01	-0.06	0.02	-0.00